ABSTRACT

Rational combinatorial computational methods use accurate quantum mechanical and molecular modeling techniques to identify optimum polymerization catalysts for polar olefins. Using mechanistic information to model the polymerization reaction, the methods systematically vary components of a catalyst template to calculate a potential energy surface for a number of catalyst candidates. The potential energy surfaces are compared to identify a catalyst for the catalytic polymerization reaction. Internal Lewis acid single site polar olefin polymerization catalyst compositions and compounds for polymerizing polar olefins are also described.

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